

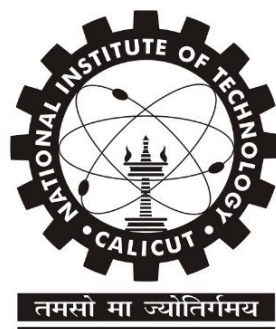
Operatorial Approaches to Classical Mechanics

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Submitted in partial fulfilment for the award of
the degree of Bachelor of Technology in Engineering Physics

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CERTIFICATE

This is to certify that the report titled "Operatorial Approaches to Classical Mechanics" is a bonafide record of the major project done by Eldhose Benny(B200147EP) and Janani Gomathi R(B200137EP) under my supervision and guidance, in partial fulfilment of the requirements for the award of Degree of Bachelor of Technology in Engineering Physics from National Institute of Technology Calicut for the year 2023-24.

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I declare that this project report titled **Operatorial Approaches to Classical Mechanics** submitted in partial fulfilment of the degree of **B.tech in Engineering Physics** is a record of original work carried out by me under the supervision of **Dr. P.N. Bala Subramanian** and has not formed the basis of any other degree or diploma, in this or any other Institution or University. In keeping with the ethical practice of reporting scientific information, due acknowledgements have been made wherever the findings of others have been cited.

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1 Koopman von Neumann Mechanics

1.1 Introduction

Several attempts have been made to approach classical mechanics in ways that are different from Newtonian Mechanics. Over time, we moved to mathematically more complex Lagrangian and Hamiltonian formulations which have given us a deep understanding of the symmetry, mathematical structures, etc. of classical dynamical systems. Meanwhile, the development of Quantum Mechanics presented the need to develop yet another approach to classical mechanics. This is because Quantum Mechanics has a mathematical structure that is unique and different from the one used to describe classical physics. The change in the mathematical structure during the transition from the microscopic world (the quantum world) to the macroscopic world (the classical world) proves to be a challenge.

The need to study the interplay between quantum and classical mechanics motivated the attempts to express both theories in mathematical formalisms that are similar to each other. For this, one could either rewrite Quantum mechanics to the language of classical mechanics or put classical Hamiltonian mechanics in the same mathematical language of quantum mechanics. Koopman-von-Neumann (KvN) mechanics arose as a result of attempts to formulate both classical and quantum mathematical formalism on the same basis of Hilbert spaces. While the usual classical mechanics is formulated in the phase space framework with observables being functions of position, momentum and time, the KvN approach to classical mechanics starts with the introduction of a Hilbert Space of complex and square-integrable functions. Further, the modulus square of these wave functions will be equal to the probability density in phase space and the observables are defined to be operators. Even when we use operatorial language, one must note that KvN formalism still deals with classical systems where position and momentum can be measured simultaneously. Further, unlike the quantum mechanical wave function, the modulus and phase of the KvN wave function evolve separately.

Redefining the classical problems using KvN mechanics gives new perspectives on the foundations of quantum theory. The common framework also makes KvN mechanics the most suitable tool for solving systems where there is an interplay between classical and quantum systems. Moreover, KvN gives a convincing explanation for the emergence of classicality from

Quantum Mechanics. If we start from the representation of quantum mechanics in the phase space instead of configuration space, it can be shown that the KvN equation naturally arises from the quantum picture in the classical limit. Besides, the KvN theory has also been used to derive purely classical results. Unlike in the quantum theory the Phase and the Amplitude evolve separately. Now, we find the dynamical equation in KvN formalism using the Liouville Theorem. In Liouville Theorem we consider a quantity $\rho = |\psi(x, p)|^2$, which is the probability density. It is a non-negative real quantity interpreted as the statistical probability that we will find a particle with momentum p , and position x , at time t .

1.2 Axioms of Koopman-von Neumann Mechanics

Now, we introduce the set of axioms followed by Koopman- von Neumann formalism [1].

1. Dynamical Equation:

$$\begin{aligned} i\frac{\partial\psi}{\partial t} &= i\left(-\frac{\partial H}{\partial p}\frac{\partial\psi}{\partial x} + \frac{\partial H}{\partial x}\frac{\partial\psi}{\partial p}\right) \\ &= \hat{L}\psi \end{aligned}$$

where \hat{L} is the Liouville Operator.

2. Normalisation: The wave function for an individual system satisfies:

$$\langle\Psi(t)|\Psi(t)\rangle = 1$$

3. Observables: They are defined by Hermitian Operators. The expectation value of an observable \hat{A} at time t is given by:

$$\langle A(t)\rangle = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle$$

4. Born rule: The probability of measuring the eigenvalue a of an observable \hat{A} at time t is given by:

$$Pr(a) = |\Pi_a |\Psi\rangle|^2$$

where Π_a is the projection onto the eigenspace of \hat{A}

5. Composite systems: The composite systems are described by tensor product in Hilbert space.

While the axioms used are the same as those in the quantum theory, a key difference is that in the classical theory, the position and momentum operators commute. That is,

$$[\hat{x}, \hat{p}] = 0. \quad (1)$$

The consequence of this difference is the introduction of two more Hermitian Operators, $\hat{\lambda}_x$ and $\hat{\lambda}_p$.

1.3 Defining $\hat{\lambda}_x$ and $\hat{\lambda}_p$

Since KvN talks about classical systems, we can demand that Newton's equations for the expectation values of observables for the expectation values of x and p to be of the form:

$$\begin{aligned} \frac{d}{dt} \langle \hat{x} \rangle &= \langle \hat{p}/m \rangle \\ \frac{d}{dt} \langle \hat{p} \rangle &= \langle -\hat{U}'(x) \rangle \end{aligned}$$

$$\begin{aligned} \frac{d}{dt} \langle \hat{x} \rangle &= \frac{d}{dt} \langle \Psi(t) | \hat{x} | \Psi(t) \rangle = \left(\frac{d}{dt} \langle \Psi(t) | \right) \hat{x} | \Psi \rangle + \langle \Psi(t) | \hat{x} \left(\frac{d}{dt} | \Psi(t) \rangle \right) \\ &= i \langle \Psi(t) | [\hat{L}, \hat{x}] | \Psi(t) \rangle \quad (2) \\ &= i \langle \Psi(t) | \frac{\hat{p}}{m} | \Psi(t) \rangle \end{aligned}$$

From this, we have the operator equation,

$$i[\hat{L}, \hat{x}] = \frac{\hat{p}}{m}$$

Similarly,

$$i[\hat{L}, \hat{p}] = -\hat{U}'(x)$$

If \hat{L} is a function of \hat{x} and \hat{p} alone, it is not possible to have the above relations. So, with the help of Stone's theorem, we introduce two additional Hermitian operators $\hat{\lambda}_x$ and $\hat{\lambda}_p$ with the relations,

$$\begin{aligned} [\hat{x}, \hat{\lambda}_q] &= i \\ [\hat{p}, \hat{\lambda}_p] &= i \end{aligned} \quad (3)$$

We can find the form of λ_x and λ_p to be:

$$\begin{aligned} \hat{\lambda}_p &\longrightarrow -i \frac{\partial}{\partial \hat{p}} \\ \hat{\lambda}_x &\longrightarrow -i \frac{\partial}{\partial \hat{x}} \end{aligned}$$

Now the Liouville Operator becomes:

$$\hat{L} = \frac{\hat{p}}{m} \hat{\lambda}_x - \widehat{U'(x)} \hat{\lambda}_p$$

2 Free Particle

2.1 Dynamics of ρ

Hamiltonian of free particle :

$$\hat{H} = \frac{\hat{p}^2}{2m} \quad (4)$$

For this Hamiltonian, the Liouville operator simplifies as:

$$\begin{aligned} \hat{L} &= i \left(-\frac{\partial H}{\partial p} \frac{\partial \psi}{\partial q} + \frac{\partial H}{\partial q} \frac{\partial \psi}{\partial p} \right) \\ &= -i \frac{\hat{p}}{m} \frac{\partial}{\partial q} \end{aligned} \quad (5)$$

If we want to diagonalize \hat{L} , we must diagonalize \hat{p} and $-i \frac{\partial}{\partial q}$ simultaneously (this can be done because $[\hat{p}, \hat{\lambda}_q] = 0$.)

Eigenstates of \hat{p} , if p_0 is an arbitrary eigenvalue:

$$\delta(p - p_0) \quad (6)$$

Eigenstates of $-i \frac{\partial}{\partial q}$, for an arbitrary real eigenvalue λ_q :

$$\frac{1}{\sqrt{2\pi}} \exp[i\lambda_q q] \quad (7)$$

The eigenstates of \hat{L} are thus the product of both eq(14) and eq(15) [2]

$$\phi(q, p) = \frac{1}{\sqrt{2\pi}} \exp[i\lambda_q q] \delta(p - p_0) \quad (8)$$

where the eigenvalues are $\epsilon = \frac{Pp_0}{m}$. From the Liouville theorem:

$$i \frac{\partial \phi}{\partial t} = \hat{L} \phi \quad (9)$$

we write :

$$\phi(q, p, t) = \frac{1}{\sqrt{2\pi}} \exp[i\lambda_q q] \delta(p - p_0) \exp[-i\lambda_q \frac{p}{m} t] \quad (10)$$

To get a wave function $\psi(q, p, 0)$ we need to write it as the superposition of Liouvillian operator \hat{L} eigenstates.

$$\begin{aligned}\psi(q, p, 0) &= \langle q, p | \Psi(0) \rangle \\ \langle q, p | \Psi(0) \rangle &= \int \int d\lambda_q dp \langle q, p | \lambda_q p \rangle \langle \lambda_q p | \Psi(0) \rangle \\ &= \int \int d\lambda_q dp \langle q, p | \lambda_q p \rangle \phi(q, p, 0)\end{aligned}\quad (11)$$

let $\langle q, p | \lambda_q, q \rangle = C(\lambda_q, p)$

$$\begin{aligned}\psi(p, q, 0) &= \int \int d\lambda_q dp C(\lambda_q, p) \exp[i\lambda_q q] \delta(p - p_0) \\ \psi(q, p, t) &= \int \int d\lambda_q dp C(\lambda_q, p) \exp[i\lambda_q q] \delta(p - p_0) \exp[-i\lambda_q \frac{p}{m} t] \\ \psi(q, p, t) &= \int \int d\lambda_q dp C(\lambda_q, p) \exp[i\lambda_q (q - \frac{p}{m} t)] \delta(p - p_0)\end{aligned}\quad (12)$$

Now let us consider the following initial wave function which is a Gaussian in q ,

$$\begin{aligned}\psi(q, p, 0) &= \frac{1}{\sqrt{\sqrt{\pi}a}} \exp[-\frac{q^2}{2a^2}] \delta(p - p_0) \\ \int \int d\lambda_q dp C(\lambda_q, p) \exp[i\lambda_q q] \delta(p - p_0) &= \frac{1}{\sqrt{\sqrt{\pi}a}} \exp[-\frac{q^2}{2a^2}] \delta(p - p_0)\end{aligned}\quad (13)$$

This wavefunction at any time t is,

$$\begin{aligned}\psi(q, p, t) &= \int \int d\lambda_q dp C(\lambda_q, p) \exp[i\lambda_q (q - \frac{p}{m} t)] \delta(p - p_0) \\ \psi(q, p, t) &= \frac{1}{\sqrt{\sqrt{\pi}a}} \exp[-\frac{1}{2a^2} (q - \frac{p}{m} t)^2] \delta(p - p_0)\end{aligned}\quad (14)$$

If we take the square of the modulus of the KvN wave $|\psi(q, p, t)|^2 = \rho(q, p, t)$, i.e., the probability of finding the particle with a position q and momentum p at time t for the wave function (22)

$$\rho(q, p, t) = \rho(q - \frac{pt}{m}, p, 0) \quad (15)$$

2.2 Spreading of the Free Particle Wave function

From equation (23) we see that the position of the wave function at a time t has displaced by distance $\frac{pt}{m}$ and the wave function moves with a group

velocity $\frac{p}{m}$. This is visible by looking at the expectation value of the position and momentum operator.

The expectation value of position i.e., \bar{q} is,

$$\bar{q} = \int dq dp q |\psi(q, p, t)|^2 = \frac{p_i t}{m} \quad (16)$$

The expectation value of momentum is,

$$\bar{p} = \int dq dp p |\psi(q, p, t)|^2 = p_i \quad (17)$$

One of the key differences between KvN Mechanics from Quantum Mechanics is that the modulus and phase of the KvN wave evolve separately.[3] In quantum mechanics, we see that the phase intermixes with modulus and the initially localised wave gets distorted at a later time t . But this is not the case for a KvN wave where the wave function remains localised at any time t . The mean square deviation for the position of the KvN wave is given by:

$$\overline{(\Delta q)^2} = (q - \bar{q})^2 \quad (18)$$

The mean square deviation of the wave function of the eq (22) at time $t=0$:

$$\overline{(\Delta q(0))^2} = \frac{a^2}{2} \quad (19)$$

The mean square deviation at time t is given by,

$$\overline{(\Delta q(t))^2} = \frac{a^2}{2} \quad (20)$$

This shows that the modulus and phase of a KvN wave evolve separately.

3 Harmonic Oscillator

The Hamiltonian of Harmonic Oscillator is given by,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{q}^2 \quad (21)$$

On substituting the potential for HO, the Liouville operator becomes:

$$\hat{L} = \frac{\hat{p}\hat{\lambda}_q}{m} + m\omega^2 \hat{q}\hat{\lambda}_p \quad (22)$$

It is not possible to find common eigenstates for the above Liouville operator as the operators \hat{p}, \hat{Q} and \hat{q}, \hat{Q} do not commute. This can be solved by plugging in the following canonical transformations:

$$\hat{q} = \hat{q}_1 \otimes I + I \otimes \hat{q}_2 = \hat{q}_1 + \hat{q}_2 \quad (23)$$

similarly,

$$\hat{\lambda}_p = \frac{1}{2}(\hat{q}_1 - \hat{q}_2) \quad (24)$$

$$\hat{p} = \hat{p}_1 - \hat{p}_2 \quad (25)$$

$$\hat{\lambda}_q = \frac{1}{2}(\hat{p}_1 + \hat{p}_2) \quad (26)$$

Substituting in (30),

$$\hat{L} = \frac{\hat{p}_1^2}{2m} + \frac{m\omega^2 \hat{q}_1^2}{2} + \left(-\frac{\hat{p}_2^2}{2m} - \frac{m\omega^2 \hat{q}_2^2}{2}\right) = \hat{H}_1 \otimes I + I \otimes \hat{H}_2. \quad (27)$$

which resemblances a system of a pair of positive and negative-mass oscillators which are uncoupled.

Note: The intermediate variables p_1, p_2, q_1, q_2 have the following commutation relations:

$$[\hat{q}_1, \hat{p}_1] = i, [\hat{q}_2, \hat{p}_2] = i \quad (28)$$

The eigenvalue equation of the Liouville operator can be written as follows:

$$\hat{L} |n, m\rangle = \hat{H}_1 |n\rangle + \hat{H}_2 |m\rangle = (E_n + E_m) |n, m'\rangle \quad (29)$$

Now, let us try to solve H_1 and H_2 separately.

3.1 Solving \hat{H}_1

$$\hat{H}_1 |n\rangle = E_n |n\rangle \quad (30)$$

Defining ladder operators:

$$\hat{a} = \frac{1}{\sqrt{2}}(\sqrt{m\omega} \hat{q}_1 + i \frac{\hat{p}_1}{\sqrt{m\omega}}) \quad (31)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\sqrt{m\omega} \hat{q}_1 - i \frac{\hat{p}_1}{\sqrt{m\omega}}) \quad (32)$$

$$\hat{N} = \hat{a}^\dagger \hat{a} \quad (33)$$

Now,

$$\hat{H}_1 = \hbar\omega(\hat{N} + \frac{1}{2}) \quad (34)$$

Eigenstates of H_1 are found by solving for the usual Harmonic Oscillator. Eigenstates are $|n\rangle$ where $n=0,1,2,\dots$ and the Eigenvalues $E_n = (n + \frac{1}{2})\hbar\omega$. Further, any $|n\rangle$ can be written as:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n |0\rangle}{\sqrt{n!}} \quad (35)$$

3.2 Solving for \hat{H}_2

$$\hat{H}_2 |m'\rangle = E_m |m'\rangle \quad (36)$$

Defining ladder operators:

$$\hat{b} = \frac{1}{\sqrt{2}}(\sqrt{m\omega}\hat{q}_2 + i\frac{\hat{p}_2}{\sqrt{m\omega}}) \quad (37)$$

$$\hat{b}^\dagger = \frac{1}{\sqrt{2}}(\sqrt{m\omega}\hat{q}_2 - i\frac{\hat{p}_2}{\sqrt{m\omega}}) \quad (38)$$

$$\hat{M} = -\hat{b}^\dagger \hat{b} \quad (39)$$

$$\begin{aligned} \hat{M} - \frac{1}{2} &= -\hat{b}^\dagger \hat{b} - \frac{1}{2} \\ &= -\frac{1}{2}(\sqrt{m\omega}\hat{q}_2 + i\frac{\hat{p}_2}{\sqrt{m\omega}})(\sqrt{m\omega}\hat{q}_2 - i\frac{\hat{p}_2}{\sqrt{m\omega}}) - \frac{1}{2} \\ &= -\frac{m\omega\hat{q}_2^2}{2} - \frac{\hat{p}_2^2}{2m\omega} = \frac{H_2}{\omega}. \end{aligned} \quad (40)$$

$$H_2 = \omega(\hat{M} - \frac{1}{2}) \quad (41)$$

Also,

$$[H_2, \hat{M}] = 0$$

Therefore, $|m\rangle$ are the simultaneous eigenstates of H_2 and \hat{M} .

3.2.1 Finding the range of m

$$\langle m | \hat{M} | m \rangle = -\langle m | \hat{b}^\dagger \hat{b} | m \rangle = -|b | m \rangle|^2 \leq 0.$$

$$\langle m | \hat{M} | m \rangle = m \langle m | m \rangle = m$$

Therefore $m \leq 0$. For convenience let $m = -m'$, which means $m \geq 0$ and

$$\hat{M} | -m \rangle = -m | -m \rangle, m = 0, 1, 2, \dots$$

3.2.2 Finding action of \hat{b} and \hat{b}^\dagger on $|-m\rangle$

$$\begin{aligned} [\hat{M}, \hat{b}] &= \hat{b} \\ [\hat{M}, \hat{b}^\dagger] &= -\hat{b}^\dagger \end{aligned} \quad (42)$$

$$\begin{aligned} \hat{M}\hat{b}|-m\rangle &= (-m+1)\hat{b}|-m\rangle \\ \hat{M}\hat{b}^\dagger|-m\rangle &= (-m-1)\hat{b}^\dagger|-m\rangle \end{aligned} \quad (43)$$

Therefore we can say that $\hat{b}|-m\rangle$ and $\hat{b}^\dagger|-m\rangle$ are eigenstates of \hat{M} .

$$\begin{aligned} \hat{b}|-m\rangle &= c_-|-m+1\rangle \\ \hat{b}^\dagger|-m\rangle &= c_+|-m-1\rangle \end{aligned} \quad (44)$$

We can find $c_- = \sqrt{m}$ and $c_+ = \sqrt{m+1}$.

$$\begin{aligned} \hat{b}|-m\rangle &= \sqrt{m}|-m+1\rangle \\ \hat{b}^\dagger|-m\rangle &= \sqrt{m+1}|-m-1\rangle \end{aligned} \quad (45)$$

3.2.3 Eigenstates and Eigenvalues of \hat{H}_2

$$\begin{aligned} \hat{b}^\dagger|-m-1\rangle &= \sqrt{m}|-m\rangle \\ |-m\rangle &= \frac{\hat{b}^\dagger|-(m-1)\rangle}{\sqrt{m}} \\ &= \frac{(\hat{b}^\dagger)^m|-(m-m)\rangle}{\sqrt{m}\sqrt{m-1}\dots\sqrt{1}} \\ |-m\rangle &= \frac{(\hat{b}^\dagger)^m|0\rangle}{\sqrt{m!}} \end{aligned} \quad (46)$$

Now, the energy eigenstate becomes,

$$\begin{aligned} H_2|-m\rangle &= E_m|-m\rangle \\ &= \omega\left(\hat{M} - \frac{1}{2}\right)|-m\rangle \\ &= \omega\left(-m - \frac{1}{2}\right)|-m\rangle \end{aligned}$$

Therefore,

$$E_m = -m - \frac{1}{2}, m = 0, 1, 2, \dots \quad (47)$$

3.3 Back to the composite system

Finding the eigenvalues of the composite system,

$$\begin{aligned}
\hat{H} |n, m\rangle &= E |n, m\rangle \\
\hat{H}_2 |n\rangle \otimes I |m\rangle + I |n\rangle \otimes \hat{H}_2 |m\rangle &= E |n, m\rangle \\
(n + \frac{1}{2})\omega |n, m\rangle + (-m - \frac{1}{2})\omega |n, m\rangle &= E |n, m\rangle \\
E &= (n + \frac{1}{2} - m - \frac{1}{2})\omega \\
E &= (n - m)\omega
\end{aligned} \tag{48}$$

3.4 Expressing the ground state $|00\rangle$ in $|q, p\rangle$ basis

The lowering operators, \hat{a} and \hat{b} when acted on the ground state $|00\rangle$ gives 0.

$$\begin{aligned}
(\hat{a} \otimes I + I \otimes \hat{b}) |00\rangle &= (\sqrt{m\omega}(q_1 \otimes I) + \frac{i(I \otimes p_1)}{\sqrt{m\omega}}) + \\
&(\sqrt{m\omega}(I \otimes q_2) + \frac{i(p_2 \otimes I)}{\sqrt{m\omega}})
\end{aligned} \tag{49}$$

Here,

$$\begin{aligned}
q_1 \otimes I &= \frac{q + 2\lambda_p}{2} \\
I \otimes q_2 &= \frac{q - 2\lambda_p}{2} \\
p_1 \otimes I &= \frac{p + 2\lambda_q}{2} \\
I \otimes p_2 &= \frac{2\lambda_q - p}{2}
\end{aligned} \tag{50}$$

Substituting in (57), we get,

$$(\sqrt{m\omega}\hat{q} + i\frac{2\hat{\lambda}_q}{\sqrt{m\omega}}) |00\rangle = 0 \tag{51}$$

$$\begin{aligned}
\langle qp | \int \int dq' dp' |q'p'\rangle \langle q'p' | (\sqrt{m\omega}\hat{q} + i\frac{2\hat{\lambda}_q}{\sqrt{m\omega}}) |00\rangle &= 0 \\
\int \int dq' dp' \langle qp | q'p'\rangle (\sqrt{m\omega} \langle q'p' | \hat{q} |00\rangle + i\frac{2}{\sqrt{m\omega}} \langle q'p' | \hat{\lambda}_q |00\rangle) &= 0 \\
&= \sqrt{m\omega}q\psi_{00}(q,p) + 2\sqrt{\frac{1}{m\omega}}\frac{\partial}{\partial q}\psi_{00}(q,p) = 0. \\
\frac{\partial}{\partial q}\psi_{00}(q,p) &= -\frac{m\omega}{2}q\psi_{00}(q,p)
\end{aligned} \tag{52}$$

Similarly,

$$(\hat{a} \otimes I - I \otimes \hat{b}) |00\rangle = 0$$

and we obtain,

$$\frac{\partial}{\partial p}\psi_{00}(q,p) = \frac{-p}{2m\omega}\psi_{00}(q,p) \tag{53}$$

Simultaneous solution of (44) and (45) is:

$$\psi_{00}(q,p) = A \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega})$$

Normalising,

$$\psi_{00}(q,p) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega})$$

3.5 General State $|nm\rangle$ in $|q,p\rangle$ basis

Finding $|10\rangle$

$$\begin{aligned}
|10\rangle &= (\hat{a}^\dagger \otimes I) |00\rangle \\
&= (\sqrt{m\omega}(\frac{\hat{q} + 2\hat{\lambda}_p}{2}) - i(\frac{\hat{p} + 2\hat{\lambda}_q}{2})\frac{1}{\sqrt{m\omega}}) |00\rangle \\
\langle qp | 10\rangle &= \langle qp | \int \int dq' dp' |q'p'\rangle \langle q'p' | (\sqrt{m\omega}(\frac{\hat{q} + 2\hat{\lambda}_p}{2}) - i(\frac{\hat{p} + 2\hat{\lambda}_q}{2})\frac{1}{\sqrt{m\omega}}) |00\rangle \\
\psi_{10}(q,p) &= \int \int dq' dp' \langle qp | q'p'\rangle (\sqrt{m\omega}(\frac{q}{2} + i\frac{\partial}{\partial p})) - i(\frac{p}{2} - i\frac{\partial}{\partial q})\frac{1}{\sqrt{m\omega}} \langle q'p' | 00\rangle \\
&= \sqrt{m\omega}\frac{q}{2} - \frac{ip}{2\sqrt{m\omega}} - \frac{ip}{2\sqrt{m\omega}} + \sqrt{m\omega}\frac{q}{2} \psi_{00} \\
\psi_{10} &= (\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}}) \psi_{00} \\
\psi_{10}(q,p) &= \frac{1}{\sqrt{2\pi}} (\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}}) \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega}) \tag{54}
\end{aligned}$$

Finding $|01\rangle$

$$|01\rangle = (I \otimes \frac{\hat{b}^\dagger}{\sqrt{1!}}) |00\rangle$$

Carrying out calculations similar to the previous section,

$$\psi_{01}(q, p) = (\sqrt{m\omega}q + \frac{ip}{\sqrt{m\omega}})\psi_{00} \quad (55)$$

Finding $|11\rangle, |20\rangle, |02\rangle$

$$|11\rangle = (\frac{\hat{a}^\dagger}{\sqrt{1!}} \otimes I) |01\rangle$$

$$\psi_{11}(q, p) = (\sqrt{m\omega}q + \frac{ip}{\sqrt{m\omega}})(\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}})\psi_{00} \quad (56)$$

Similarly,

$$\psi_{20}(q, p) = \frac{1}{\sqrt{2!}}(\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}})^2\psi_{00}(q, p) \quad (57)$$

$$\psi_{02}(q, p) = \frac{1}{\sqrt{2!}}(\sqrt{m\omega}q + \frac{ip}{\sqrt{m\omega}})^2\psi_{00}(q, p) \quad (58)$$

Finally, $|mn\rangle$

Deducing the pattern in the above states,

$$\psi_{nm}(q, p) = \frac{1}{\sqrt{2\pi}\sqrt{m!n!}}(\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}})^n(\sqrt{m\omega}q + \frac{ip}{\sqrt{m\omega}})^m\psi_{00}(q, p) \quad (59)$$

3.6 Verification of the eigenstates using delta functions

Consider an initial wavefunction: $\psi(0) = \delta(q - q_0)\delta(p - p_0)$ Now, the coefficient of $\psi(0)$ is given as,

$$\begin{aligned}
C_{nm}(0) &= \langle \psi_{nm} | \psi \rangle = \int dq dp \langle \psi_{nm} | qp \rangle \langle qp | \psi \rangle = \int dq dp \psi_{nm}^* \psi(q, p, 0) \\
&= \int dq dp \frac{1}{\sqrt{2\pi m!n!}} (\sqrt{m\omega}q + \frac{ip}{\sqrt{m\omega}})^n (\sqrt{m\omega}q - \frac{ip}{\sqrt{m\omega}})^m \\
&\quad \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega}) \delta(q - q_0) \delta(p - p_0) \\
&= \frac{1}{\sqrt{2\pi m!n!}} \int dq dp \sum_k^n \sum_r^m \binom{n}{k} \binom{m}{r} (\sqrt{m\omega}q)^{n+m-k-r} (\frac{ip}{\sqrt{m\omega}})^{k+r} (-1)^r \\
&\quad \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega}) \delta(q - q_0) \delta(p - p_0) \\
&= \frac{1}{\sqrt{2\pi m!n!}} \binom{n}{k} \sqrt{m\omega} q_0^{n-k} (\frac{ip_0}{\sqrt{m\omega}})^k \binom{m}{r} (\sqrt{m\omega} q_0)^{m-r} (\frac{-ip_0}{\sqrt{m\omega}})^r \\
&\quad \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega}) \\
&= \frac{1}{\sqrt{2\pi m!n!}} (\sqrt{m\omega} q_0 + \frac{ip_0}{\sqrt{m\omega}})^n (\sqrt{m\omega} q_0 - \frac{ip_0}{\sqrt{m\omega}})^m \\
&\quad \exp(-\frac{m\omega q_0^2}{4}) \exp(-\frac{p_0^2}{4m\omega})
\end{aligned}$$

The wave function at any time t is given by $\psi(t) = e^{-iLt}\psi(0)$.

Now, let us find the coefficient of the time-evolved wave function.

$$\begin{aligned}
C_{nm}(t) &= \langle \psi_{nm} | e^{-iLt} | \psi(0) \rangle = \langle \psi_{nm} | e^{-i(n-m)\omega t} | \psi(0) \rangle \\
&= \int dq dp \langle \psi_{nm} | e^{-i(n-m)\omega t} | qp \rangle \langle qp | \psi(0) \rangle \\
&= \int dq dp e^{-i(n-m)\omega t} \psi_{nm}^* \psi(q, p, 0) \\
&= \int dq dp e^{-i(n-m)\omega t} \frac{1}{\sqrt{2\pi m!n!}} \\
&\quad \sum_k^n \binom{n}{k} (\sqrt{m\omega}q)^{n-k} (\frac{ip}{\sqrt{m\omega}})^k \sum_r^m \binom{m}{r} (\sqrt{m\omega}q)^{m-r} (\frac{-ip}{\sqrt{m\omega}})^r \\
&\quad \exp(-\frac{m\omega q^2}{4}) \exp(-\frac{p^2}{4m\omega}) \delta(p - p_0) \delta(q - q_0)
\end{aligned}$$

The previous analysis shows that coefficient takes the form,

$$C_{nm}(t) = \frac{1}{\sqrt{2\pi m!n!}} (\sqrt{m\omega}q_0 + \frac{ip_0}{\sqrt{m\omega}})^n (\sqrt{m\omega}q - \frac{ip_0}{\sqrt{m\omega}})^m \exp(-\frac{m\omega q_0^2}{4}) \exp(-\frac{p_0^2}{4m\omega}) \exp(-i(n-m)\omega t) \quad (60)$$

For $p_0 = 0$, let us substitute,

$$e^{-i(n-m)\omega t} = (\sin(\omega t) - i\cos(\omega t))^n (\sin(\omega t) + i\cos(\omega t))^m$$

$$C_{nm}(t) = \frac{1}{\sqrt{2\pi m!n!}} (\sqrt{m\omega}q_0(\sin\omega t - i\cos\omega t))^n (\sqrt{m\omega}q(\sin\omega t + i\cos\omega t))^m \exp(-\frac{m\omega q_0^2}{4}) \quad (61)$$

From Newtonian mechanics, the solution of harmonic oscillator with initial momentum as zero is:

$$q = q_0 \cos\omega t$$

$$p = -m\omega q_0 \sin\omega t$$

Therefore, the expected wavefunction at time t is ,

$$\psi(t) = \delta(q - q_0 \cos\omega t) \delta(p + m\omega q_0 \sin\omega t) \quad (62)$$

Component of this wavefunction in the eigenstates of the Liouvillian is:

$$\begin{aligned} C_{nm} &= \langle \psi_{nm} | \psi \rangle = \int dq dp \langle \psi_{nm} | qp \rangle \langle qp | \psi \rangle \\ &= \int dq dp \frac{1}{\sqrt{2\pi m!n!}} (\sqrt{m\omega}q_0(\sin\omega t - i\cos\omega t))^n (\sqrt{m\omega}q(\sin\omega t + i\cos\omega t))^m \\ &\quad \exp(-\frac{m\omega q_0^2}{4}) \exp(-\frac{m\omega p_0^2}{4}) \delta(q - q_0 \cos\omega t) \delta(p + m\omega q_0 \sin\omega t) \end{aligned} \quad (63)$$

This simplifies as,

$$C_{nm}(t) = \frac{1}{\sqrt{2\pi n!m!}} (\sqrt{m\omega}q_0(\cos\omega t - i\sin\omega t))^n (\sqrt{m\omega}q_0(\cos\omega t + i\sin\omega t))^m \exp(-\frac{m\omega q_0^2}{4}) \quad (64)$$

This matches with the expression for $C_{nm}(t)$ we have found earlier, thus verifying our results.

4 Galilei Group

4.1 Introduction

Representations using the Galilei group have been realised in both classical and quantum mechanics, although the approaches taken for the two are quite different. The Hilbert space formalism of quantum mechanics naturally leads to a study of the unitary representations of Galilei group. However, the derivation of classical mechanics from the structure of the Galilei group has been in the context of canonical representation in terms of Poisson brackets in Hamiltonian Mechanics [4].

Unlike the KvN theory, we derive an operational formulation of classical mechanics from a unitary, irreducible representation of the Galilei group. Also, this approach is independent of any previous results from analytical mechanics. First, the complex Hilbert space is postulated and the Galilei group is realised such that space-time transformations are represented by unitary transformations acting on the complex space. By direct construction, this can be proved to be compatible with the basic postulates of classical mechanics and that KvN theory is its particular case.

4.2 Lie Algebra

The Galilei group is a ten-parameter group that consists of space and time translations, rotations and pure Galilei transformation (boosts). The general transformation $(\vec{x}, t) \longrightarrow (\vec{x}', t)$ can be written as

$$\begin{aligned}\vec{x}' &= R\vec{x} + \vec{b}t + \vec{a}, \\ t' &= t + \tau,\end{aligned}$$

where R is rotation, \vec{a} is a space displacement, \vec{b} is the velocity of a moving frame and τ is a time displacement.

The generators of the basic group transformations will be associated with Hermitian operators as follows: \mathcal{J}_α stands for the rotations around α -axis ($\alpha = 1, 2, 3$); $\hat{\lambda}_\alpha$ is the space displacement generator in the α - direction; \mathcal{G}_α correspond to the Galilean boost along the α - axis; \hat{L} will be the time displacement generator. All these operators will act on a suitable Hilbert space.

The space-time transformation of the Galilei group will be realised by unitary operators with the following convention:

Space-Time Transformations Unitary Operators

Rotations

$$\vec{x} \longrightarrow R_\alpha(\theta_\alpha)\vec{x} \qquad e^{-i\theta_\alpha\hat{\mathcal{J}}_\alpha}$$

Displacement

$$\vec{x} \longrightarrow \vec{x} + \vec{a} \qquad e^{-ia_\alpha\hat{\lambda}_{x_\alpha}}$$

Galilean Boost

$$\vec{x} \longrightarrow \vec{x} + \vec{b}t \qquad e^{-ib_\alpha\hat{\mathcal{G}}_\alpha}$$

Time Displacement

$$t' \longrightarrow t + \tau \qquad e^{i\tau\hat{L}}$$

The commutator relations of the group are as follows:

$$\begin{aligned} [\hat{\lambda}_{x_\alpha}, \hat{\lambda}_{x_\beta}] &= 0, \\ [\hat{\mathcal{G}}_\alpha, \hat{\mathcal{G}}_\beta] &= 0 \\ [\hat{\mathcal{J}}_\alpha, \hat{\mathcal{J}}_\beta] &= i\epsilon_{\alpha\beta\gamma}\hat{\mathcal{J}}_\gamma, \\ [\hat{\mathcal{J}}_\alpha, \hat{\lambda}_{x_\beta}] &= i\epsilon_{\alpha\beta\gamma}\hat{\lambda}_{x_\gamma}, \\ [\hat{\mathcal{J}}_\alpha, \hat{\mathcal{G}}_\beta] &= i\epsilon_{\alpha\beta\gamma}\hat{\mathcal{G}}_\gamma, \\ [\hat{\mathcal{G}}_\alpha, \hat{\lambda}_{x_\beta}] &= i\delta_{\alpha\beta}\mathcal{M}, \\ [\hat{\mathcal{J}}_\alpha, \hat{L}] &= 0, \\ [\hat{\mathcal{G}}_\alpha, \hat{L}] &= i\hat{\lambda}_{x_\alpha}, \\ [\hat{\lambda}_{x_\alpha}, \hat{L}] &= 0 \end{aligned} \tag{65}$$

Here, \mathcal{M} is the central charge of the algebra, quite different from its counterpart in the representation of Quantum Mechanics using the Galilei group.

4.3 Classical representation of the Galilei algebra

We consider that the position \hat{r} and momentum \hat{p} of a point particle can be simultaneously measured with arbitrary accuracy. Due to this lack of uncertainty principle between position and momentum, the vector in Hilbert space is of the form,

$$|\psi\rangle = \int \langle r, p|\psi\rangle |r, p\rangle dr dp, \tag{66}$$

such that $\psi(r, p) = \langle r, p|\psi\rangle$ is a square-integrable function and the kets obey orthonormality. The probability of finding the particle with position r and momentum p is given by the Born's rule.

The geometrical effect of $\hat{\lambda}_r$, $\hat{\mathcal{G}}$ and $\hat{\mathcal{J}}$ are translation in space coordinates, a Galilean boost, and a rotation respectively. Accordingly the action of these operators on base kets are as follows:

$$\begin{aligned} e^{-i\vec{a} \cdot \hat{\lambda}_r} |\vec{r}, \vec{p}\rangle &= |\vec{r} + \vec{a}, \vec{p}\rangle, \\ e^{i\vec{b} \cdot \hat{\mathcal{G}}} |\vec{r}, \vec{p}\rangle &\propto |\vec{r} + \vec{b}t, \vec{p} + \vec{b}\rangle, \\ e^{-i\theta \hat{n} \cdot \hat{\mathcal{J}}} |\vec{r}, \vec{p}\rangle &= |\vec{r} + \theta \hat{n} \times \vec{r}, \vec{p} + \theta \hat{n} \times \vec{p}\rangle \end{aligned} \quad (67)$$

The proportionality sign in the 2nd equation indicates that a phase factor can be present due to the above-mentioned commutation relations.

Now we introduce position and momentum operators $\hat{R} = (\hat{X}_1, \hat{X}_2, \hat{X}_3)$ and $\hat{P} = (\hat{P}_1, \hat{P}_2, \hat{P}_3)$ such that by definition, we have

$$\begin{aligned} \hat{X}_\alpha |\vec{r}, \vec{p}\rangle &= x_\alpha |\vec{r}, \vec{p}\rangle, \\ \hat{P}_\alpha |\vec{r}, \vec{p}\rangle &= p_\alpha |\vec{r}, \vec{p}\rangle. \end{aligned} \quad (68)$$

We will also assume the existence of operators $\hat{\lambda}_p = (\hat{\lambda}_{p1}, \hat{\lambda}_{p2}, \hat{\lambda}_{p3})$ that act as translation operators in the momentum coordinates,

$$e^{-\vec{b} \cdot \hat{\lambda}_p} |\vec{r}, \vec{p}\rangle = |\vec{r}, \vec{p} + \vec{b}\rangle. \quad (69)$$

As $\hat{\lambda}_{x_\alpha}$ and $\hat{\lambda}_{p_\alpha}$, they are conjugated in the quantum sense to \hat{X}_α and \hat{P}_α respectively. The following commutation relations are postulated,

$$\begin{aligned} [\hat{X}_\alpha, \hat{X}_\beta] &= [\hat{X}_\alpha, \hat{P}_\beta] = [\hat{P}_\alpha, \hat{P}_\beta] = 0 \\ [\hat{X}_\alpha, \hat{\lambda}_{p\beta}] &= [\hat{P}_\alpha, \hat{\lambda}_{x\beta}] = 0 \\ [\hat{X}_\alpha, \hat{\lambda}_{x\beta}] &= i\delta_{\alpha\beta} \\ [\hat{P}_\alpha, \hat{\lambda}_{p\beta}] &= i\delta_{\alpha\beta} \end{aligned} \quad (70)$$

Now, we postulate the same dynamical relation between the position operator \hat{X}_α and \hat{P}_α as in quantum mechanics,

$$\begin{aligned} \frac{d}{dt} \langle \hat{R} \rangle &= \frac{\langle \hat{P} \rangle}{m}, \\ \frac{\hat{P}}{m} &= i[\hat{L}, \hat{R}], \\ \frac{d}{dt} \langle \hat{P} \rangle &= m \langle \hat{a} \rangle \end{aligned} \quad (71)$$

where \hat{a} is the acceleration operator. Now, we demand that $\hat{a} = \hat{a}(\hat{R}, \hat{P})$ and it is independent of $\hat{\lambda}_p$ and $\hat{\lambda}_r$. Therefore,

$$i[\hat{L}, \hat{P}] = \hat{F}(\hat{R}, \hat{P}) \quad (72)$$

where \hat{F} is an arbitrary function and m is the mass of the particle.

The set of six operators (\hat{R}, \hat{P}) form a complete set of commuting operators in the Hilbert space of a single classical particle. Therefore, due to our defined commutation relations and Schur's lemma, the collection of $(\hat{R}, \hat{P}, \hat{\lambda}_r, \hat{\lambda}_p)$ forms an irreducible set of operators on the Hilbert space of the square-integrable wave functions, $\psi(\vec{r}, \vec{p}) = \langle \vec{r}, \vec{p} | \psi \rangle$. Now we will use these commutation relations and the set-up to evaluate free particle and harmonic oscillator.'

4.4 Free Particle

We have seen that the Liouvillian of Free Particle is:

$$\hat{L} = \frac{\hat{p}_x}{m} \hat{\lambda}_x \quad (73)$$

And the equation of motion will be,

$$\frac{d\hat{p}_x}{dt} = i[\hat{L}, \hat{p}_x] = 0 \quad (74)$$

which implies that \hat{p}_x is a constant of motion. Also,

$$\begin{aligned} \frac{d\hat{x}}{dt} &= i[\hat{L}, \hat{x}] \\ i\frac{\hat{p}_x}{m}[\hat{\lambda}_x, \hat{x}] &= \frac{\hat{p}_x}{m} \end{aligned} \quad (75)$$

The state will evolve with time as,

$$\begin{aligned} \psi(x, p_x, 0) &\longrightarrow \psi(x, p_x, t) = \langle x, p_x | \hat{U}(t) | \psi(0) \rangle \\ \langle x, p_x | e^{-t\hat{L}} | \psi(0) \rangle &= \langle x, p_x | e^{-it\frac{\hat{p}_x}{m}\hat{\lambda}_x} | \psi(0) \rangle \\ &= \langle x + \frac{p_x}{m}t, p_x | \psi(0) \rangle \\ \langle x, p_x | \psi(t) \rangle &= \psi(x - \frac{p_x}{m}t, p_x, 0) \end{aligned} \quad (76)$$

4.5 Harmonic Oscillator

Now we move to the Harmonic Oscillator, whose Liouvillian was found to be,

$$\hat{L} = \frac{\hat{p}_x^2 \hat{\lambda}_x}{m} - m\omega^2 \hat{x} \hat{\lambda}_{p_x} \quad (77)$$

Let us define,

$$\begin{aligned}\hat{p}'_x &= \frac{\hat{p}_x}{m\omega} \\ \hat{\lambda}'_{\hat{p}_x} &= m\omega \hat{\lambda}_{\hat{p}_x}\end{aligned}$$

Applying these transformations to the Liouvillian,

$$\hat{L} = \omega(\hat{p}'_x \hat{\lambda}_x - \hat{x} \hat{\lambda}_{\hat{p}_x}) \quad (78)$$

Now, consider the following commutation relations,

$$\begin{aligned}i[\hat{L}, \hat{x}] &= \hat{p}_x \\ i[\hat{L}, \hat{p}_x] &= \hat{x}.\end{aligned} \quad (79)$$

From these relations, we see that this follows the same commutation relation as the z-component of angular momentum with position operators \hat{x} and \hat{y} . Using this analogy, we can say that \hat{L} acts as the generator of rotation in the phase space with the perpendicular axis \hat{x} and \hat{p}_x .

We define the evolution operator to be:

$$\hat{U}(t) = e^{-i\hat{L}t} = e^{-i\omega t(\hat{p}_x \hat{\lambda}_x - \hat{x} \hat{\lambda}_{\hat{p}_x})} \quad (80)$$

The action of this operator on the state $|x_0, 0\rangle$ is given as,

$$\hat{U}(t) |x_0, 0\rangle = |x_0 \cos \omega t, -m\omega x_0 \sin \omega t\rangle$$

Evolving the state with initial position x_0 and momentum 0,

$$\begin{aligned}\psi(x, 0, 0) &\longrightarrow \psi(\hat{x}, \hat{p}_x, t) \\ &= \langle x_0, 0 | \hat{U}(t) | \psi(0) \rangle = \langle x_0, 0 | e^{-i\hat{L}t} | \psi(0) \rangle \\ &= \langle x_0 \cos \omega t, -m\omega x_0 \sin \omega t | \psi(0) \rangle \\ &= \psi(x_0 \cos \omega t, -m\omega x_0 \sin \omega t)\end{aligned} \quad (81)$$

5 Anharmonic Oscillator

5.1 Liouvillian and general state

Consider a cubic anharmonic oscillator with potential given by:

$$U(x) = \frac{1}{2}kx^2 + \frac{\epsilon}{3}x^3 \quad (82)$$

where k is the force constant and ϵ is a very small parameter// The Hamiltonian of the system is:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2} + \frac{\epsilon^3 \hat{x}^3}{3} \quad (83)$$

The Liouvillian thus takes the form:

$$\hat{L} = \hat{p}_x \hat{\lambda}_x - m\omega^2 \hat{\lambda}_{px} - \epsilon \hat{x}^2 \hat{\lambda}_{px} \quad (84)$$

Defining:

$$\begin{aligned} \hat{p}_x' &= \frac{\hat{p}_x}{m\omega} \\ \hat{\lambda}_{px}' &= m\omega \hat{\lambda}_{px} \end{aligned} \quad (85)$$

Applying this transformations to Liouvillian:

$$\hat{L} = \omega(\hat{p}_{xx}' \hat{\lambda}_x - \hat{x} \hat{\lambda}_p' - \frac{\epsilon \hat{x}^2 \hat{\lambda}_p'}{m\omega^2}) \quad (86)$$

The evolution operator is :

$$\hat{U}(t) = \exp(-i\hat{L}t) \quad (87)$$

Using Zassenhaus formula and expanding till linear order in ϵ we get $\hat{U}(t)$ to be:

$$\hat{U}(t) = \exp(-i\omega t \hat{L}_m) \exp\left(\frac{it\epsilon \hat{x}^2 \hat{\lambda}_p'}{\omega}\right) \exp\left(-\frac{\epsilon t^2 [\hat{L}_m, \hat{x}^2 \hat{\lambda}_p']}{2}\right) \quad (88)$$

where \hat{L}_m is the Harmonic oscillator Liouvillian.

Solving the commutator $[\hat{L}_m, \hat{x}^2 \hat{\lambda}_p']$ and substituting:

$$\hat{U}(t) = \exp(-i\omega t \hat{L}_m) \exp\left(\frac{it\epsilon \hat{x}^2 \hat{\lambda}_p'}{\omega}\right) \exp\left(-\frac{\epsilon t^2 (-2i\hat{p}_x' \hat{x} \hat{\lambda}_p' + i\hat{x}^2 \hat{\lambda}_x)}{2}\right) \quad (89)$$

Action of $\hat{U}(t)$ on the state $|x_0, 0\rangle$:

$$\hat{U}(t) |x_0, 0\rangle = |x_0 \cos(\omega t) + \frac{\epsilon t^2 x_0^2}{2}, -\omega x_0^2 \sin(\omega t) + t\epsilon x_0^2\rangle \quad (90)$$

Evolving the state with initial position x_0 and momentum 0,

$$\begin{aligned} \psi(x, 0, 0) &\longrightarrow \psi(x, p_x, t) \\ &= \langle x_0, 0 | \hat{U}(t) | \psi(0) \rangle = \langle x_0, 0 | e^{-i\hat{L}t} | \psi(0) \rangle \\ &= \langle x_0 \cos(\omega t) + \frac{\epsilon t^2 x_0^2}{2}, -\omega x_0^2 \sin(\omega t) + t\epsilon x_0^2 | \psi(0) \rangle \\ &= \psi(x_0 \cos(\omega t) + \frac{\epsilon t^2 x_0^2}{2}, -\omega x_0^2 \sin(\omega t) + t\epsilon x_0^2 | \end{aligned} \quad (91)$$

5.2 Comparison with classical perturbation theory

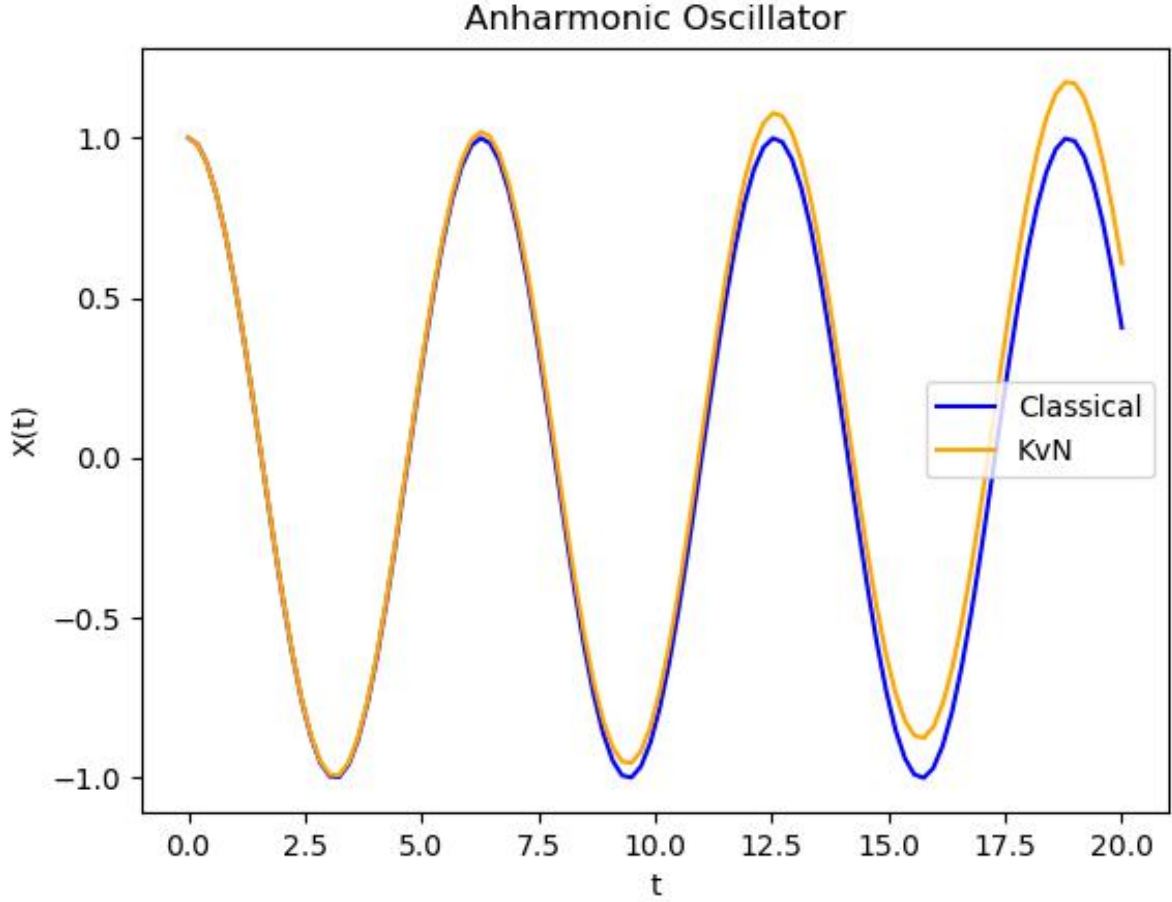


Figure 1: $m=\omega=1; \epsilon=0.001$

6 Central Potential

6.1 Finding the Liouvillian

The Hamiltonian for Central Potential is,

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{p}_\theta^2}{2m\hat{r}^2} + \hat{V}(r) \quad (92)$$

where $\hat{V}(r) = k\hat{r}^n$ Accordingly, we find the Liouvillian in cartesian coordinates to be:

$$\hat{L} = i\left(\frac{\partial H}{\partial x} \frac{\partial}{\partial p_x} - \frac{\partial H}{\partial p_x} \frac{\partial}{\partial x} + \frac{\partial H}{\partial y} \frac{\partial}{\partial p_y} - \frac{\partial H}{\partial p_y} \frac{\partial}{\partial y}\right) \quad (93)$$

Transforming \hat{L} from cartesian coordinates to polar coordinates [5],

$$\begin{aligned}
L = & i \left(\frac{\partial H}{\partial x} \frac{\partial H}{\partial p_x} - p_x \frac{\partial H}{\partial p_x} \frac{\partial}{\partial x} + \frac{\partial H}{\partial y} \frac{\partial H}{\partial p_y} - \frac{\partial H}{\partial p_y} \frac{\partial}{\partial y} \right) \\
= & i \left[\left(\frac{\partial H}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial H}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial H}{\partial p_r} \frac{\partial p_r}{\partial x} + \frac{\partial H}{\partial p_\theta} \frac{\partial p_\theta}{\partial x} \right) \left(\frac{\partial}{\partial p_r} \frac{\partial p_r}{\partial p_x} + \frac{\partial}{\partial p_\theta} \frac{\partial p_\theta}{\partial p_x} \right) \right. \\
& - \left(\frac{\partial H}{\partial p_r} \frac{\partial p_r}{\partial p_x} + \frac{\partial H}{\partial p_\theta} \frac{\partial p_\theta}{\partial p_x} \right) \left(\frac{\partial r}{\partial x} + \frac{\partial \theta}{\partial x} + \frac{\partial p_r}{\partial x} + \frac{\partial p_\theta}{\partial x} \right) \\
& + \left(\frac{\partial H}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial H}{\partial \theta} \frac{\partial \theta}{\partial y} + \frac{\partial H}{\partial p_r} \frac{\partial p_r}{\partial y} + \frac{\partial H}{\partial p_\theta} \frac{\partial p_\theta}{\partial y} \right) \left(\frac{\partial}{\partial p_r} \frac{\partial p_r}{\partial p_y} + \frac{\partial}{\partial p_\theta} \frac{\partial p_\theta}{\partial p_y} \right) \\
& \left. - \left(\frac{\partial H}{\partial p_r} \frac{\partial p_r}{\partial p_y} + \frac{\partial H}{\partial p_\theta} \frac{\partial p_\theta}{\partial p_y} \right) \left(\frac{\partial r}{\partial y} + \frac{\partial \theta}{\partial y} + \frac{\partial p_r}{\partial y} + \frac{\partial p_\theta}{\partial y} \right) \right] \quad (94)
\end{aligned}$$

The partial derivatives are of the form:

$$\begin{aligned}
\frac{\partial r}{\partial x} &= \cos\theta \quad \left| \quad \frac{\partial \theta}{\partial x} = \frac{\sin\theta}{r} \quad \left| \quad \frac{\partial p_r}{\partial x} = \frac{p_\theta \sin\theta}{r^2} \quad \left| \quad \frac{\partial p_\theta}{\partial x} = \frac{p_\theta \cos\theta}{r} \right. \right. \\
\frac{\partial r}{\partial y} &= \sin\theta \quad \left| \quad \frac{\partial \theta}{\partial y} = \frac{\cos\theta}{r} \quad \left| \quad \frac{\partial p_r}{\partial y} = \frac{p_\theta \cos\theta}{r^2} \quad \left| \quad \frac{\partial p_\theta}{\partial y} = \frac{p_\theta \sin\theta}{r} \right. \right. \\
\frac{\partial r}{\partial p_x} &= 0 \quad \left| \quad \frac{\partial \theta}{\partial p_x} = 0 \quad \left| \quad \frac{\partial p_r}{\partial p_x} = \cos\theta \quad \left| \quad \frac{\partial p_\theta}{\partial p_x} = -r \sin\theta \right. \right. \\
\frac{\partial r}{\partial p_y} &= 0 \quad \left| \quad \frac{\partial \theta}{\partial p_y} = 0 \quad \left| \quad \frac{\partial p_r}{\partial p_y} = \sin\theta \quad \left| \quad \frac{\partial p_\theta}{\partial p_y} = r \cos\theta \right. \right.
\end{aligned}$$

On substitution and on the condition that \hat{H} is cyclic in θ for central potential systems the Liouvillian operator becomes:

$$\begin{aligned}
\hat{L} = & i \left[\left(\cos\theta \frac{\partial H}{\partial r} - \frac{p_\theta \sin\theta}{r^2} \frac{\partial H}{\partial p_r} + \left(\frac{p_\theta \cos\theta}{r} + p_r \sin\theta \right) \frac{\partial H}{\partial p_\theta} \right) \right. \\
& \left(\cos\theta \frac{\partial}{\partial p_r} - r \sin\theta \frac{\partial}{\partial p_\theta} \right) \\
& - \left(\cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r} \frac{\partial}{\partial \theta} - \frac{p_\theta \sin\theta}{r^2} \frac{\partial}{\partial p_r} + \left(\frac{p_\theta \cos\theta}{r} + p_r \sin\theta \right) \frac{\partial}{\partial p_\theta} \right) \\
& \left(\cos(\theta) \frac{\partial H}{\partial p_r} - r \sin(\theta) \frac{\partial H}{\partial p_\theta} \right) \\
& + \left(\sin\theta \frac{\partial H}{\partial r} + \frac{p_\theta \sin\theta}{r^2} \frac{\partial H}{\partial p_r} + \left(\frac{p_\theta \sin\theta}{r} - p_r \cos\theta \right) \frac{\partial H}{\partial p_\theta} \right) \\
& \left(\sin\theta \frac{\partial}{\partial p_r} + r \cos\theta \frac{\partial}{\partial p_\theta} \right) \\
& - \left(\sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r} \frac{\partial}{\partial \theta} + \frac{p_\theta \cos\theta}{r^2} \frac{\partial}{\partial p_r} + \left(\frac{p_\theta \sin\theta}{r} - p_r \cos\theta \right) \frac{\partial}{\partial p_\theta} \right) \\
& \left. \left(\sin\theta \frac{\partial H}{\partial p_r} + r \cos\theta \frac{\partial H}{\partial p_\theta} \right) \right] \quad (95)
\end{aligned}$$

On expanding the terms and simplification we get:

$$\hat{L} = -\frac{\partial H}{\partial p_r} \frac{\partial}{\partial r} - \frac{\partial H}{\partial p_\theta} \frac{\partial}{\partial \theta} - \frac{\partial H}{\partial r} \frac{\partial}{\partial p_r} \quad (96)$$

We define the generators of \hat{r} , $\hat{\theta}$, \hat{p}_r and \hat{p}_θ to be,

$$\begin{aligned} \hat{\lambda}_r &= i \frac{\partial}{\partial r} & \hat{\lambda}_{p_r} &= i \frac{\partial}{\partial p_r} \\ \hat{\lambda}_\theta &= i \frac{\partial}{\partial \theta} & \hat{\lambda}_{p_\theta} &= i \frac{\partial}{\partial p_\theta} \end{aligned}$$

Thereby, we can find the commutation relations,

$$\begin{aligned} [\hat{r}, \hat{\lambda}_r] &= i & [\hat{\theta}, \hat{\lambda}_\theta] &= i \\ [\hat{p}_r, \hat{\lambda}_{p_r}] &= i & [\hat{p}_\theta, \hat{\lambda}_{p_\theta}] &= i \end{aligned}$$

Substituting the Hamiltonian for central potential along the above-mentioned relations, Liouvillian becomes:

$$\hat{L} = -\frac{\hat{p}_r \hat{\lambda}_r}{m} - \frac{\hat{p}_\theta \hat{\lambda}_\theta}{m \hat{r}^2} + \left(-\frac{\hat{p}_\theta}{m \hat{r}^3} + n k \hat{r}^{n-1}\right) \hat{\lambda}_{p_r} \quad (97)$$

6.2 Dynamics of observables

Now, we find the dynamics of observables, $\hat{r}, \hat{\theta}, \hat{p}_r, \hat{p}_\theta$,

$$\frac{d\hat{p}_\theta}{dt} = i[\hat{L}, \hat{p}_\theta] = 0 \quad (98)$$

Hence p_θ is a constant of motion and angular momentum is conserved as expected.

$$\begin{aligned} \frac{d\hat{p}_r}{dt} &= i[\hat{L}, \hat{p}_r] \\ &= i\left[\left(-\frac{\hat{p}_\theta^2}{m \hat{r}^3} + n k \hat{r}^{n-1}\right) \hat{\lambda}_{p_r}, \hat{p}_r\right] \\ &= i\left(-\frac{\hat{p}_\theta^2}{m \hat{r}^3} + n k \hat{r}^{n-1}\right) [\hat{\lambda}_{p_r}, \hat{p}_r] \\ &= i\left(-\frac{\hat{p}_\theta^2}{m \hat{r}^3} + n k \hat{r}^{n-1}\right) \end{aligned} \quad (99)$$

Now, finding the dynamics of \hat{r} ,

$$\begin{aligned} \frac{d\hat{r}}{dt} &= i[\hat{L}, \hat{r}] \\ &= -i \frac{\hat{p}_r}{m} [\hat{\lambda}_r, \hat{r}] \\ &= \frac{\hat{p}_r}{m} \end{aligned} \quad (100)$$

Finally, the dynamics of $\hat{\theta}$ goes as,

$$\begin{aligned}\frac{d\hat{\theta}}{dt} &= -i[\hat{L}, \hat{\theta}] \\ &= -i\left[\frac{\hat{p}_\theta}{m\hat{r}^2}\hat{\lambda}_\theta, \hat{\theta}\right] \\ &= \frac{\hat{p}_\theta}{m\hat{r}^2}\end{aligned}\tag{101}$$

The found dynamics of observables match with the expected dynamics from a classical central potential system.

7 Conclusion

The objective of the project was to study various operatorial approaches to classical mechanics. We started with understanding the foundations of Koopman- von Neumann Mechanics and the key differences in its operatorial language that set it apart from Quantum Mechanics. We then used the KvN formalism to evaluate the free particle and successfully mapped it back to the Newtonian free particle. Next, we solved for the general eigenstates ψ_{nm} of Liouvillian in the Harmonic Oscillator system. We also verified the credibility of the found eigenstates.

The next operatorial approach was derived from the irreducible representation of the Galilei group. We studied the postulated Lie Algebra of the group and re-examined Free particle and Harmonic Oscillator using this approach. Here, we found that the results match with those found using the KvN approach. With this, we confirmed that the two approaches are indeed equivalent.

Then, we studied the Anharmonic Oscillator with cubic perturbation. We found the general states with linear order approximation. Further, we compared the evolution of the found state in time with the state found through using classical perturbation theory. Finally, we moved on to examine the Central Potential system where we first found the Liouvillian in polar coordinates. Then we calculated the dynamics of all observables of the system and saw that angular momentum is conserved as expected.

In the future, we aim to further study the central potential system and anharmonic oscillator. We would like to find ways to better approximate the general state of anharmonic oscillator using perturbative approach.

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